Spectral Integration and Two-Point Boundary Value Problems

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A numerical method for two-point boundary value problems with constant coefficients is developed which is based on integral equations and the spectral integration matrix for Chebyshev nodes. The method is stable, achieves superalgebraic convergence, and requires $O(N \log N)$ operations, where N is the number of nodes in the discretization. Although stable spectral methods have been constructed in the past, they have generally been based on reformulating the recurrence relations obtained through spectral differentiation in an attempt to avoid the ill-conditioning introduced by that process.

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1 Introduction

Spectral methods are now a popular tool for the solution of many types of partial differential equations. In the usual formulation, the basic idea is to represent the solution f by means of a (truncated) series expansion, and to compute spatial derivatives of f by analytic differentiation of the series. The linear map $\mathcal{D}_N$ which takes a vector of N function values $\{f(x_i)\}$ to a vector of N derivative values $\{f'(x_i)\}$ is known as the spectral differentiation matrix. The precise form of $\mathcal{D}_N$ depends on the location of the points $\{x_i\}$ and the choice of the approximating series. For periodic functions, Fourier series are used with the function tabulated at equispaced nodes. For bounded domains, Chebyshev or Legendre series are used with the function tabulated at Chebyshev or Legendre nodes, respectively.

Although spectral differentiation is remarkably accurate in exact arithmetic, there are a number of difficulties associated with its use. Ill-conditioning of the matrix with increasing N frequently causes degradation of the observed precision. Furthermore, as recently demonstrated by Trefethen and Trummer for certain hyperbolic problems [6], the time step restrictions due to this ill-conditioning can be more severe than those predicted by the standard stability theory.

In this paper, we will consider only the simplest steady-state case, namely linear two-point boundary value problems with constant coefficients. It is well known that problems of this type are efficiently and accurately solved by spectral methods. On the other hand, it is also well known that care must be taken in applying spectral methods to such problems. The naive approach leads to the use of unstable recurrence relations for the determination of the expansions coefficients, a consequence of the high condition number of $\mathcal{D}_N$.

Our main purpose in this paper is to provide a consistent framework for developing well-conditioned spectral methods. After collecting the necessary results from approximation theory, we present a fast algorithm for computing the indefinite integral of a given function by means of the *spectral integration matrix*. The indefinite integral is then used to recast the governing differential equation of the boundary value problem as an integral equation, which is solved with spectral accuracy.

2 Chebyshev Approximation

We will require several results from approximation theory. The *Chebyshev polynomial* of degree k on $[-1,1]$ is defined by the formula

$$T_k(\cos\theta) = \cos(k\theta) \ . \tag{1}$$

Clearly, $|T_k(x)| \leq 1$ for $x \in [-1,1]$,

$$T_0(x) = 1, \qquad T_1(x) = x \tag{2}$$

and, using elementary trigomometric identities,

$$T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x) \quad \text{for } k \geq 1 \ . \tag{3}$$

The functions T_k constitute an orthonormal basis with respect to the inner product

$$(f,g) = \int_{-1}^{1} f(x)g(x)(1 - x^2)^{-1/2}dx \ . \tag{4}$$

The *Chebyshev nodes* t_i of degree k are the zeros of T_k, namely

$$t_i = \cos\frac{(2i+1)\pi}{2k}\ , \quad \text{for } i = 0, 1, 2, ..., k-1\ . \tag{5}$$

Let $C^n[-1,1]$ denote the set of functions defined on $[-1,1]$ with n continuous derivatives. If $f \in C^n[-1,1]$ and

$$g(x) = \sum_{k=0}^{\infty} a_k T_k(x) \tag{6}$$

is the Chebyshev expansion associated with f, then

$$a_k = \frac{2}{\pi c_k}\int_{-1}^{1} f(x)T_k(x)(1-x^2)^{-1/2}dx \ = \frac{2}{\pi c_k}\int_0^{\pi} f(\cos\theta)\cos k\theta\, d\theta\ , \tag{7}$$

where $c_0 = 2$ and $c_k = 1$ for $k > 0$. Moreover, the remainder in truncating the series at N terms is of the order

$$O\left(\frac{1}{N^{n-1}}\right) \qquad \text{as} \quad N \to \infty\ . \tag{8}$$

In particular, if f is infinitely differentiable, then the remainder goes to zero superalgebraically (faster than any finite power of $1/N$). For a more complete discussion, see Gottlieb and Orszag [3].

Remark 2.1: In practice, the Chebyshev series (6) is truncated at some finite number of terms, say N. By relation (7), the coefficients a_k are the coefficients of the Fourier cosine series of $F(\theta) = f(\cos\theta)$. Thus, if f is tabulated at equispaced points in θ, a condition satisfied by the Chebyshev nodes $\{t_i\}$, we can obtain all N coefficients a_k by means of the FFT or, more precisely, the Fast Cosine Transform, using $O(N\log N)$ operations. Similarly, the inverse cosine transform can be used to compute function values $g(x) \approx f(x)$ at the nodes $\{t_i\}$ from the coefficients a_k of the expansion.

2.1 Differentiation and Integration of Chebyshev Expansions

Definition 2.1 *Let X be the space consisting of infinite sequences of real numbers*

$$\mathbf{x} = (x_0, x_1, x_2, ...)\ .$$

For any $\mathbf{a} \in X$, we will denote by $\mathcal{D}(\mathbf{a})$ the sequence $\mathbf{b}$ given by the formula

$$b_k = \frac{1}{c_k}\sum_{\substack{p=k+1\\ p+k\ odd}}^{\infty} p\cdot a_p \tag{9}$$

where $c_0 = 2$ and $c_k = 1$ for $k > 0$. We will refer to the mapping $\mathcal{D} : X \to X$ as spectral differentiation. We will denote by $\mathcal{I}(\mathbf{a})$ the sequence $\mathbf{d}$ given by the formulae

$$d_k = \frac{1}{2k}(c_{k-1}\cdot a_{k-1} - c_{k+1}\cdot a_{k+1}) \qquad \text{for } k \geq 1 \tag{10}$$

$$d_0 = 2\,d_1 - 2\,d_2 + 2\,d_3 - \cdots\ . \tag{11}$$

where the coefficients c_k are defined as above. We will refer to the mapping $\mathcal{I} : X \to X$ as spectral integration.

The above definitions are motivated by the following lemma, which may be found in the Appendix to [3].

Lemma 2.1 *Let f be a smooth function given by a Chebyshev series*

$$f(x) = \sum_{k=0}^{\infty} a_k T_k(x). \tag{12}$$

Then the derivative of f has a series expansion of the form

$$f'(x) = \sum_{k=0}^{\infty} b_k T_k(x) \tag{13}$$

with b_k given by (9). The integral of f has a series expansion of the form

$$\int_{-1}^{x} f(t)\,dt \;= \sum_{k=0}^{\infty} d_k T_k(x) \tag{14}$$

where d_k is given by (10) and (11).

Remark 2.2: The series expansion (14) is the basis for *Clenshaw-Curtis* quadrature [2]. After obtaining the coefficients d_k, one computes

$$\int_{-1}^{1} f(x)\,dx = 2 \sum_{k=0}^{\infty} d_{2k+1}\ , \tag{15}$$

which follows immediately from the equalities

$$T_k(-1) = (-1)^k \qquad \text{and} \qquad T_k(1) = 1\ . \tag{16}$$

It is clear from (9) and (10) that $\mathcal{D}$ is unbounded in the l_∞ norm, while $\|\mathcal{I}\|_\infty < 2$. This behavior is reflected in the condition numbers of the finite-dimensional analogs of these operators. If f is represented by a truncated Chebyshev expansion

$$f(x) = \sum_{k=0}^{N} a_k T_k(x)\ , \tag{17}$$

then the coefficients of f' are still given by (9), but the summation is truncated at N terms. Now let $\mathbf{a} = (a_0, a_1, ..., a_N)$, $\hat{\mathbf{a}} = (a_0 + \epsilon, a_1 + \epsilon, ..., a_N + \epsilon)$, $\mathcal{D}(\mathbf{a}) = \mathbf{b}$ and $\mathcal{D}(\hat{\mathbf{a}}) = \hat{\mathbf{b}}$. Then

$$\frac{\|\hat{\mathbf{b}} - \mathbf{b}\|_\infty}{\|\hat{\mathbf{a}} - \mathbf{a}\|_\infty} = O(N^2)\,, \tag{18}$$

the maximum error being incurred for the calculation of b_0. In other words, the process of differentiation via Chebyshev series has a condition number proportional to N^2. On the other hand, it is easy to show that for any $\hat{\mathbf{a}}$,

$$\frac{\|\hat{\mathbf{d}} - \mathbf{d}\|_\infty}{\|\hat{\mathbf{a}} - \mathbf{a}\|_\infty} \le \frac{3}{2}\,, \tag{19}$$

where $\mathbf{d} = \mathcal{I}(\mathbf{a})$ and $\hat{\mathbf{d}} = \mathcal{I}(\hat{\mathbf{a}})$. In other words, the process of differentiation via Chebyshev series has a condition number bounded by 2.

2.2 The Spectral Integration Matrix

The spectral differentiation matrix for Chebyshev nodes can be expressed in terms of $\mathcal{D}$ by the formula

$$\mathcal{D}_N = \mathcal{C}_N^{-1} \cdot \mathcal{D} \cdot \mathcal{C}_N \tag{20}$$

where $\mathcal{C}_N$ is the discrete cosine transform of dimension N.

Definition 2.2 *The spectral integration matrix for Chebyshev nodes $\mathcal{I}_N$ is defined by the formula*

$$\mathcal{I}_N = \mathcal{C}_N^{-1} \cdot \mathcal{I} \cdot \mathcal{C}_N \ . \tag{21}$$

It is clear that the matrix $\mathcal{I}_N$ can be applied to a vector in $O(N \log N)$ operations by using a Fast Cosine Transform algorithm.

Before turning to the solution of two-point boundary value problems, we briefly investigate the behavior of $\mathcal{D}_N$ and $\mathcal{I}_N$ with a set of three examples (Fig. 1). Note that in these examples, we test $\mathcal{D}_N$ by differentiating a function $f(x)$ and we test $\mathcal{I}_N$ by integrating the corresponding derivative $f'(x)$. The integration of $f(x)$ itself is even more stable and of less interest. When $f(x) = \sin(x)$, we observe the expected convergence as soon as the number of sampling points is sufficient, approximately π per wavelength. However, as the number of points increases, differentiation becomes less and less accurate while integration is essentially unaffected. Although there is no need to use 1000 points to resolve $\sin(x)$ alone, the error introduced by its differentiation remains when the problem becomes more complex and more points *are* required. For example, when $f(x) = \sin(x) + .01\sin(10x)$, about 50 points are required to achieve spectral accuracy, at which point an error of the order 10^{-4} has already been incurred. When $f(x) = \sin(x) + .005\sin(60x)$, the situation is worse. In single precision, even with the optimal choice of N, the mean square error is greater than 1%.

3 Two-point Boundary Value Problems

The two-point boundary value problems considered here are second order equations of the form

$$L\,u = u'' + \mu\,u' + \nu\,u = f(x)\ , \quad x \in [-1,1] \tag{22}$$

with $\mu, \nu \in \mathbf{R}$ and Dirichlet conditions

$$u(-1) = \alpha\ , \qquad u(1) = \beta\ . \tag{23}$$

The fact that high order polynomial approximations achieve superalgebraic convergence for such differential equations has been known for a long time. Ciarlet, Schultz and Varga [1] have shown that superalgebraic convergence can be achieved even when the governing ordinary differential equation is nonlinear, so long as the solution is sufficiently smooth. In the standard spectral formulation [3], using a "Chebyshev-tau" method, we seek a solution

$$u_N(x) = \sum_{k=0}^{N} a_k T_k(x)\ , \tag{24}$$

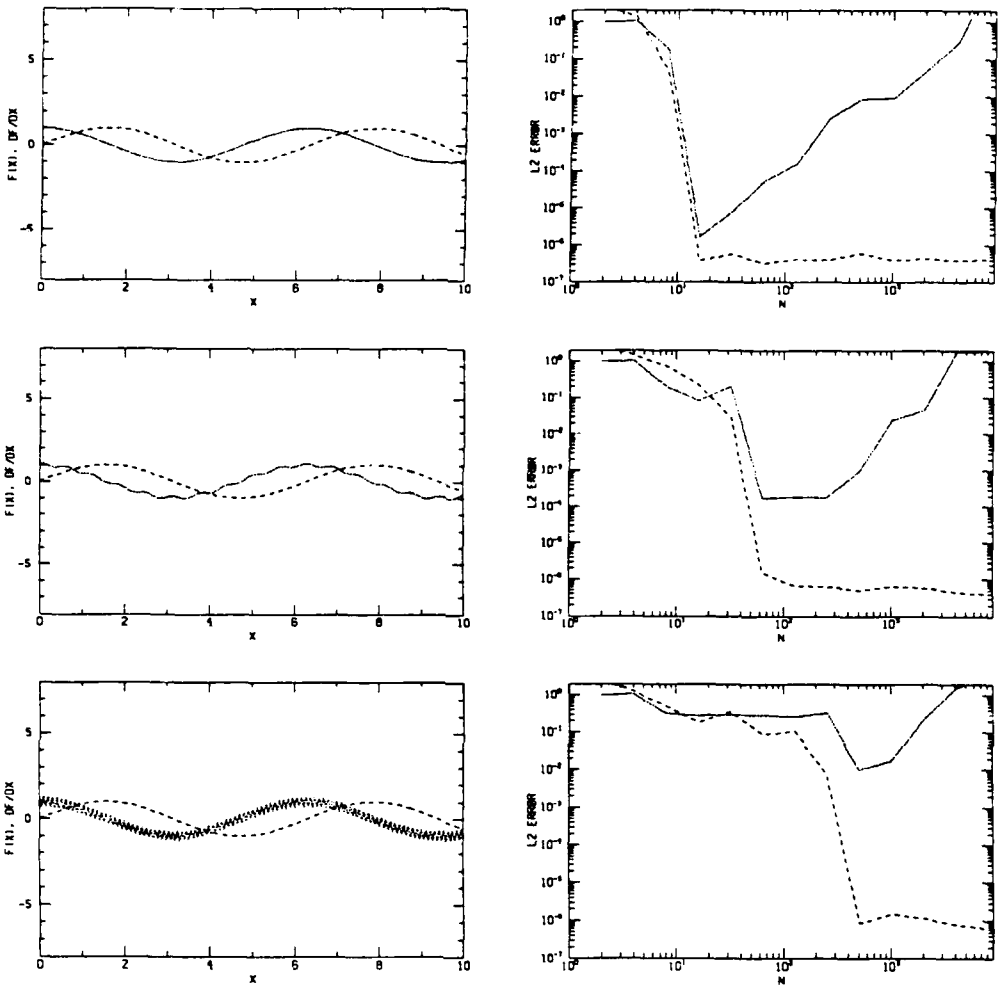

Figure 1

The numerical behavior of spectral differentiation and integration is demonstrated with three examples. The left hand of each pair of figures is a plot of $f(x)$ as a dashed curve and $f'(x)$ as a dotted curve. The right hand of each pair is a plot of the mean square error in the spectral differentiation of $f(x)$ (dotted line) and the spectral integration of $f'(x)$ (dashed line) vs. the number of points in the discretization. For the top figure $f(x) = sin(x)$, for the middle figure, $f(x) = \sin(x) + .01\sin(10x)$ and for the bottom figure $f(x) = \sin(x) + .005\sin(60x)$.

subject to the boundary conditions

$$\sum_{k=0}^{N}(-1)^k a_k = \alpha \qquad \text{and} \qquad \sum_{k=0}^{N} a_k = \beta \ , \tag{25}$$

where we have used the equalities in (15). From the differential equation (21) and the spectral differentiation matrix, we obtain the relations

$$\frac{1}{c_k} \sum_{\substack{p=k+2 \\ p+k \text{ even}}}^{N} p(p^2-k^2)a_p + \frac{\mu}{c_k} \sum_{\substack{p=k+1 \\ p+k \text{ odd}}}^{N} p a_p + \nu a_k = f_k \qquad \text{for } k = 0, ..., N-2 \tag{26}$$

where the $\{f_k\}$ are the Chebyshev expansion coefficients for the right-hand side $f(x)$. This set of equations is inherently ill-conditioned. A reformulation of the recurrence relations is, therefore, used to compute the solution in a stable manner (see [3], p. 118.).

Consider now the one-dimensional Poisson equation

$$u'' = f(x) \ , \quad u(-1) = \alpha \ , \ u(1) = \beta \ . \tag{27}$$

Rather than setting up the recurrence relations as in (25), it would be very attractive to be able to write

$$u(x) = \int_{-1}^{x} \int_{-1}^{t} f(\tau)\, d\tau \ dt \ + C_1 x + C_0 \ . \tag{28}$$

The spectral integration matrix of Definition 2 1 provides us with precisely the ability to compute this formal solution. The constants C_1 and C_0 are chosen to satisfy the boundary condition.

When the differential equation contains terms in u' or u, we still have a simple analytic expression for the solution. We may assume, without loss of generality, that we are given homogeneous boundary conditions and that the corresponding Green's function has the form

$$G(x,t) = \begin{cases} u_1(x)\, v_1(t) & \text{for } x < t \\ u_2(x)\, v_2(t) & \text{for } x > t \end{cases} \tag{29}$$

where u_1 and u_2 are solutions of the homogeneous equation $L\,u = 0$. Since the equation has constant coefficients, u_1 and u_2 are known explicitely. The desired solution can then be written as

$$u(x) = \int_{-1}^{1} G(x,t) f(t)\, dt \tag{30}$$

$$= u_1(x) \cdot \int_{-1}^{x} v_1(t) f(t)\, dt \ + \tag{31}$$

$$u_2(x) \cdot \left(\int_{-1}^{1} v_2(t) f(t)\, dt - \int_{-1}^{x} v_2(t) f(t)\, dt \right) \ . \tag{32}$$

The indefinite integrals in the preceding expression can be tabulated by means of the spectral integration matrix, while the definite integral can be computed by formula (14). Once this initial work, requiring two Fast Cosine Transforms, is done, the solution is obtained using approximately $3N$ additional operations, where N is the number of Chebyshev nodes used. A similar observation is made by Rokhlin in [4], where the integrals are computed by a finite-order quadrature formula.

His approach has the advantage that it does not depend on the location of the discretization nodes. One drawback of this particular use of Green's functions is that the terms u_1, v_1, u_2 and v_2 may behave much more violently than either the right-hand side or the solution, requiring many more points in the discretization than necessary. Another drawback is that the method does not extend to non-constant coefficient problems, since we cannot determine the Green's function analytically.

We consider a closely related approach which does not require knowledge of the Green's function. An integral equation is constructed by solving for $\sigma(x) = u''(x)$ rather than u itself. The original system (21) becomes

$$\sigma(x) + \mu \int_{-1}^{x} \sigma(t)\, dt + \mu\, C_1 + \nu \int_{-1}^{x} \int_{-1}^{t} \sigma(\tau)\, d\tau\, dt + \nu\, C_1 x + \nu\, C_0 = f(x) \tag{33}$$

Representing $\sigma(x)$ and $f(x)$ by truncated Chebyshev series

$$\sigma(x) = \sum_{k=0}^{N} a_n\, T_n(x) \qquad\qquad f(x) = \sum_{k=0}^{N} f_n\, T_n(x) \tag{34}$$

and using the spectral integration matrix, we obtain the system of equations

$$a_0 + \mu\, C_1 + \nu\, C_0 = f_0 \tag{35}$$

$$a_1 + \frac{\mu}{2}(c_0\, a_0 - c_2\, a_2) + \frac{\nu}{8}(8\, C_1 + a_1 - a_3) = f_1 \tag{36}$$

$$\cdots$$

$$a_k + \frac{\mu}{2k}(c_{k-1}\, a_{k-1} - c_{k+1}\, a_{k+1}) + \frac{\nu}{2k}(c_{k-1}\, d_{k-1} - c_{k+1}\, d_{k+1}) = f_k \tag{37}$$

$$\text{for } k = 2, ..., N\,, \tag{38}$$

where $c_0 = 2$, $c_1 = ... = c_N = 1$, $c_k = 0$ for $k > N$, and the coefficients d_k are given by equation (10). This is a system of $N+1$ equations with $N+3$ unknowns (the coefficients a_k and the constants of integration C_0 and C_1). Two additional equations are obtained from the boundary conditions

$$C_0 - C_1 + \sum_{k=2}^{N} \frac{1}{2k}(c_{k-1}\, d_{k-1} - c_{k+1}\, d_{k+1})(-1)^k = \alpha\,, \tag{39}$$

$$C_0 + C_1 + \sum_{k=2}^{N} \frac{1}{2k}(c_{k-1}\, d_{k-1} - c_{k+1}\, d_{k+1}) = \beta\,. \tag{40}$$

The discrete problem is pentadiagonal except for the two rows derived from the boundary conditions, and can be solved using approximately $10N$ floating point operations.

4 Numerical Examples

A two-point boundary value problem solver, using the method of the previous section, has been implemented and tested on a variety of examples. It requires two cosine transforms and the solution of one linear system, with a total computational cost estimated at $10\,N\,(\log N + 1)$ floating point operations. All calculations cited below were carried out in double precision on a SUN 3/50 workstation with f68881 floating point accelerator.

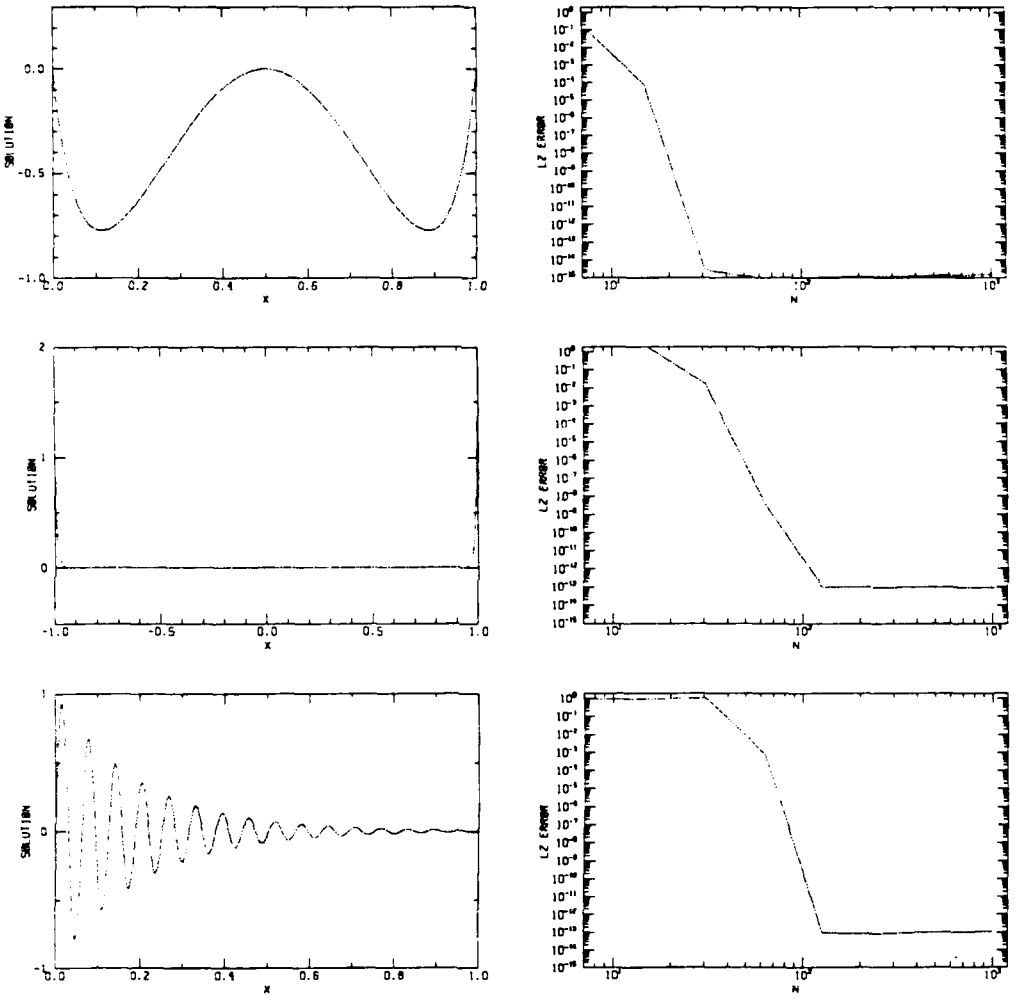

Figure 2

The numerical behavior of the integral equation algorithm, using three examples. The left hand of each pair of figures is a plot of the exact solution as a function of x. The right hand of each pair is a plot of the mean square error in the computed solution vs. the number of points in the discretization. The governing differential equations are discussed in the text.

• **Table 1**

Table of CPU times (in seconds) and mean square errors in computing the solutions to three boundary value problems. The subscripts 1-3 refer to the three equations discussed in the text and displayed graphically in Fig. 2 from top to bottom.

N	T_1	E_1	T_2	E_2	T_3	E_3
16	0.08	$7.2\ 10^{-5}$	0.06	2.2	0.06	0.9
64	0.30	$8.7\ 10^{-16}$	0.32	$4.0\ 10^{-9}$	0.32	$7.9\ 10^{-4}$
256	1.46	$1.1\ 10^{-15}$	1.48	$9.1\ 10^{-14}$	1.40	$8.1\ 10^{-14}$
1024	6.42	$1.5\ 10^{-15}$	6.32	$9.1\ 10^{-14}$	6.10	$1.0\ 10^{-13}$

The behavior of the algorithm is demonstrated with three examples (Fig. 2 and Table 1). In the first case, we used a model problem from Stoer and Bulirsch [5]

$$-y'' + 400y = -400\cos^2 \pi x - 2\pi^2 \cos 2\pi x \ , \tag{41}$$

$$y(0) = y(1) = 0 \ , \tag{42}$$

with exact solution

$$y(x) = \frac{e^{-20}}{1+e^{-20}}\, e^{20x} + \frac{1}{1+e^{-20}}\, e^{-20x} - \cos^2 \pi x \ . \tag{43}$$

Standard finite difference and finite element methods tend to converge quite slowly, due to the large derivatives of the exact solution near the boundaries. While multiple shooting, which is recommended in [5], is a viable approach, the method is computationally expensive. Our calculations show that the corresponding integral equation is solved to spectral accuracy with very little effort.

The second example involves a boundary layer near each endpoint. The governing equation is

$$\epsilon\, y'' - y = 0 \ , \tag{44}$$

$$y(-1) = 1 \ , \qquad y(1) = 2 \ , \tag{45}$$

where $\epsilon = 10^{-5}$. As is well-known, the Chebyshev nodes are particularly good at resolving boundary layers since they tend to cluster at the two endpoints (see [3]).

The third example is one where the solution is very oscillatory:

$$y'' + 5\, y' + 10000\, y = -500\cos(100x)\, e^{-5x} \ , \tag{46}$$

$$y(0) = 0 \qquad y(1) = \sin(100)\, e^{-5} \ , \tag{47}$$

for which the exact solution is

$$y(x) = \sin(100x)\, e^{-5x} \ . \tag{48}$$

In each case, it is clear that the spectral integral formulation is both rapidly convergent and stable.

5 Conclusions

The spectral integration matrix is a well-conditioned operator which yields an antiderivative of a function tabulated at Chebyshev nodes. In this paper, we have presented a fast algorithm for the solution of constant coefficient two-point boundary value problems through the use of integral equations and spectral integration. The difficulty with variable coefficient problems lies not in the formulation of the integral equation, but in the fact that the resulting system of equations for the coefficients of the Chebyshev series of u'' is dense. Gaussian elimination would require $O(N^3)$ operations, where N is the number of Chebyshev nodes used in the discretization. On the other hand, the spectral integration matrix can be used to apply the integral operator in $O(N \log N)$ operations, making iterative methods much more attractive. Rokhlin [4] has demonstrated that conjugate residual type methods can work quite well for such integral equations. The number of iterations required is a function of the underlying problem, and does not increase with the number of nodes. Unfortunately, for many situations of interest, complex behavior of the solution causes the condition number of the underlying problem and the number of iterations to be large, so that direct methods would be preferable.

I would like to thank V. Rokhlin and F. Saied for many useful discussions.

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